Critical Survey of Isoscalar and Isovector Contributions to the Spin Orbit Potential in Relativistic Mean Field Theory

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The spin-orbit (SO) interaction, emerging naturally from the Relativistic Mean Field (RMF) theory is examined critically in the light of the recently measured excitation energy differences between the terminating states built on two different configurations for nuclei belonging to the lower pf shell. The calculations are carried out using the cranked RMF framework. To further probe the iso-vector dependence of the spin-orbit potential, the energy spacing between the $g_{7/2}$ and $h_{11/2}$ states in the Sb-chain is compared to experiment. It is found that the calculation at the quantitative level deviates strongly from the experiment. In particular the balance of the iso-scalar and iso-vector strengths of the effective one body SO potential indicates that additional terms like tensor couplings may be needed to account for the experimental data.

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Low energy excitations and global properties in atomic nuclei are rather well described by the modern effective forces. Different realizations of the short range nuclear interaction have been developed, like the Skyrme and Gogny for non relativistic Hartree Fock potentials and the Relativistic Mean Field (RMF) Lagrangian, based on meson couplings. These effective theories employ a set of parameters that are adjusted to selected experimental observables in order to account for basic nuclear structure properties. Since there exist a multitude of observables and no real consensus about which of these are to be selected in a unique manner, there exist a multitude of different force parameterizations. One of the basic problems in adjusting the force parameters is related to the fact that the single particle states, that are so crucial for high accuracy calculations, are in general coupled to collective motion and therefore difficult to determine. In this context, any dataset representing single-particle motion manifests itself as an invaluable source for a rigorous test and subsequent fine-tuning of the parameters.

Recently, it was shown [1, 2] that a set of terminating states in the mass region A$\sim$ 45 may provide a unique tool to determine the strength of the spin-orbit (SO) interaction. The long experience in the studies of terminating states within the Nilsson model have clearly shown that these belong to the purest single particle states available in nuclear structure [3, 4] and hence provide an excellent laboratory for the adjustment of effective forces. Indeed, in Refs. [1, 2] it was demonstrated that for some of the Skyrme force parameterizations, the SO interaction can be adjusted in such a way, that it agrees with the experimental data, whereas some other force parameterizations can be ruled out as irreparable. The robustness of terminating states in determining properties of the nuclear energy density functional was further supported by the recent comparative study between the fully correlated shell model and the Skyrme Hartree-Fock (SHF) [5], showing essentially a one to one correspondence.

Since the SO potential emerges naturally within the RMF [6], it becomes highly interesting and important to carry out a critical survey of the SO interaction within the RMF framework, in the light of the recently measured terminating states in the lower pf shell.

In addition, there is a long standing debate on the isovector strength of the SO potential for different Skyrme parameterizations, exemplified in the recent extension [7] of the Skyrme SO potential, which needs to be confronted to experiment. Similarly, in the RMF, there is an open question as to what extend the Hartree potential that generates the SO field is sufficient to account for the experimental data or whether additional terms or constraints, e.g. tensor coupling [8] need to be added in the theoretical framework.

One may also consider the Fock terms involving the π meson, which strongly affect the effective one body SO potential [9]. In this work, we carry out a systematic investigation of the SO potential by comparison to the recent data from the lower pf shell within the framework of the cranked RMF (c-RMF) [10, 11]. To further address the iso-vector dependence of the SO potential, we employ the recently studied $g_{7/2} - h_{11/2}$ spacing, E^{gh}, in the chain of Sb isotopes [12].

Recently, experimental data on the terminating states in the lower pf shell has been reported in the literature [13, 14, 15, 16, 17, 18, 19, 20]. The terminating states considered here involve the $f_{7/2}^n$ as well as the $d_{3/2}^{-1}f_{7/2}^{n+1}$ configurations where n denotes the number of valence particles outside the ^{40}Ca core and the particle hole excitation across the magic gap 20 is of proton type. Summary of the relevant experimental results is presented in Table I. Following the discussion in Refs. [1, 2], we extract the difference, ΔE, between the excitation

TABLE I: Summary of experimental results on terminating states in lower pf shell.

	$f_{7/2}^n$			$d_{3/2}^{-1}f_{7/2}^{n+1}$			
Nucleus	I_{max}	E_{max} (MeV)	Ref.	I_{max}	E_{max} (MeV)	Ref.	ΔE (MeV)
^{42}Ca	6^+	3.189	[13]	11^-	8.297	[13]	5.108
^{44}Ca	8^+	5.088	[14]	13^-	10.568	[14]	5.480
^{44}Sc	11^+	3.567	[15]	15^-	9.141	[15]	5.574
^{45}Sc	$23/2^-$	5.417	[16]	$31/2^+$	11.022	[16]	5.605
^{45}Ti	$27/2^-$	7.144	[17]	$33/2^+$	13.028	[18]	5.884
^{46}Ti	14^+	10.040	[19]	17^-	15.550	[19]	5.510
^{47}V	$31/2^-$	10.004	[20]	$35/2^+$	15.259	[20]	5.255

energies of the states terminating within the $d_{3/2}^{-1}f_{7/2}^{n+1}$ and $f_{7/2}^n$ configurations. The value of ΔE depends predominantly on the size of the magic gap 20 which in turn directly relates to the strength of the SO potential. Within the spherical Nilsson Hamiltonian [21] the magic gap $\Delta e_{20} = \hbar\omega_o(1 - 6\kappa - 2\kappa\mu)$, depends on three major factors: i) the bulk properties of the potential characterized by $\hbar\omega_o$, ii) the strength of the SO term κ and iii) the flat-bottom and surface properties entering through the orbit-orbit term, $\sim \mu$. All three terms influence the magic gap 20 with a well defined hierarchy. For light nuclei one can disregard the flat-bottom effect ($\mu \sim 0$). Note that the smaller the energy spacing between $1d_{3/2}$ and $1f_{7/2}$, the larger the effective SO potential.

The width of the Nilsson potential, $\hbar\omega_o$, is fitted to nuclear radii. Hence, it sets a common energy scale for all microscopic models in low energy nuclear physics. Consequently, any adjustments of, in particular, the RMF parameters leading effectively even to small variations in $\hbar\omega_o$ in light nuclei is expected to endanger the good agreement already achieved between the theory and the experiment for radii and binding energies in heavy nuclei. Therefore, the difference in the excitation energies provides a unique testing ground for the SO interaction usually employed in the mean field calculations.

These simple arguments are strongly supported by the self-consistent SHF calculations [1, 2]. In particular, in Ref. [1] it is shown that the difference between the SHF and the corresponding experimental values of ΔE, averaged over all the available data, i.e. the quantity which measures the quality of the parametrization is directly correlated with the isoscalar-effective-mass scaled strength (true strength) of the iso-scalar SO interaction. This result not only exemplifies the role of the SO potential but also shows that for physical observables like ΔE (or E^{gh}) the impact of non-local effects (effective mass) on the HF single-particle spectra is, as expected, compensated by the effective coupling constants in the energy density functional.

In the RMF theory, the point nucleons are assumed to be interacting only via the c-number electromagnetic (e.m.) and the σ, ω and ρ meson fields. Within the standard nonlinear (σ, ω, ρ) interaction Lagrangian [22, 23] the SO potentials for protons and neutrons (U_{ls}^p and U_{ls}^n) can be expressed in terms of iso-scalar and iso-vector contributions as (see, for example, [24]):

$$U_{ls}^{p(n)}(\vec{r}) = \frac{1}{rm^2m^{\star 2}}\left[\left(C_\sigma^2 + C_\omega^2\right)\nabla_r\rho(\vec{r}) \pm C_\rho^2\nabla_r\rho_{pn}(\vec{r})\right]. \quad (1)$$

Here, m ($m^\star$) is the nucleon (effective) mass; the constants C_i ($i = \sigma, \omega, \rho$) are defined as $C_i = mg_i/m_i$, m_i being the meson masses; $\rho(\vec{r})$ is the total nucleon density (sum of neutron and proton densities) and $\rho_{pn}(\vec{r})$ is the difference between proton and neutron densities. Sign + (-) arises for protons (neutrons). Clearly, the iso-scalar term of the SO interaction is dominant in comparison with the iso-vector term. This can be substantiated further by examining the ratio of iso-scalar to iso-vector strengths of the SO potential in Equation (1). For NL1 [25] and NL3 [26] Lagrangian parameter sets, this ratio turns out to be 16.54 and 19.62, respectively. For Lagrangian parameter sets with density dependent couplings, DD-ME1 [27] and DD-ME2 [28], this ratio is typically around 20 or even larger. Further insight into the properties of the SO potential can be gained by assuming that proton and neutron densities have the same shape. In this case, Equation (1) reduces to:

$$U_{ls}^{p(n)} = \frac{-(C_\sigma^2 + C_\omega^2)A}{rm^2m^{\star 2}}\left[1 \mp \lambda\frac{N-Z}{A}\right]g(r) \quad (2)$$

Here, $-g(r)$ is the derivative of the density, and is negative definite; and $\lambda = C_\rho^2/(C_\sigma^2 + C_\omega^2)$. As expected, the spin orbit potential decreases (increases) for protons (neutrons) as $N - Z$ increases. However, in contrast to non-relativistic models, the iso-vector strength, λ, is at least an order of magnitude smaller, and is not an independent quantity that can be adjusted further.

In this work, we solve the c-RMF equations using the basis expansion technique [22]. The upper and lower components of Dirac spinor as well as the meson and e.m. fields are expanded in terms of three dimensional harmonic oscillator basis. We use 8 fermionic and 10 bosonic shells. We have explicitly checked for a few representative cases that the use of 10 fermionic and 10 bosonic shells produces essentially the same values of ΔE. Since primary focus is on relative quantities like ΔE, inclusion of

a larger number of shells does not alter the conclusions drawn. Further, pairing correlations are ignored. This is justified, since it is expected that the pairing correlations are quenched for the states considered here [3, 4]. Currents are crucial for the calculation of ΔE and are taken into account appropriately. For further technical details of the c-RMF model, see [10, 11]. The calculation are carried out using two frequently used parameter sets, NL1 [25] and NL3 [26]. In the calculation of E^{gh}, we also employ the RMF model with density dependent meson - nucleon couplings [27, 28, 29] using the Lagrangian parameter set DD-ME2 [28]. Preliminary results of the present calculation may be found in Ref. [30].

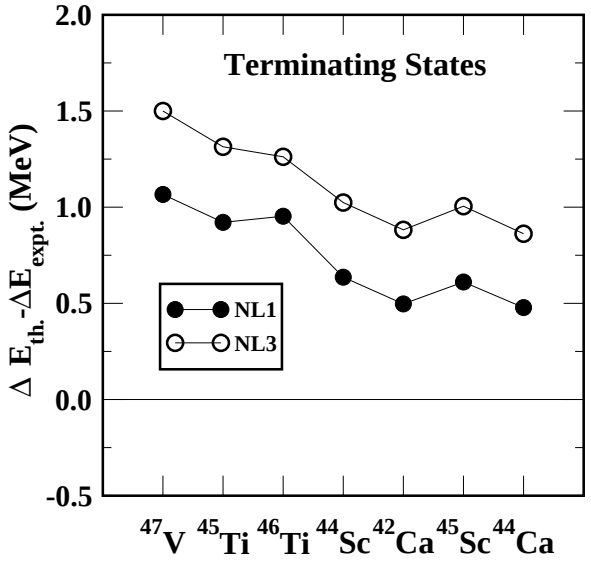

FIG. 1: The difference between theoretical and the corresponding experimental values of the excitation energy differences (ΔE) for the terminating states within the $d_{3/2}^{-1} f_{7/2}^{n+1}$ and $f_{7/2}^{n}$ configurations.

The difference between the calculated and the corresponding experimental values of ΔE is plotted in Figure 1. It is clear that ΔE values obtained using the parameter sets, NL1 and NL3, though qualitatively in agreement with the experiment, differ from each other and from the experiment. Both over-estimate the experiment. The deviation is in general larger than the corresponding Skyrme calculations. Both NL1 and NL3 values exhibit similar systematics and differ from each other roughly by 0.5 MeV on the average. Further, the NL1 values are found to be closer to the experiment than those obtained by using set NL3, with mean squared deviations 0.59 and 1.31 respectively. Apparently, the magnitude of the iso-scalar spin orbit potential is at variance with experiment. It should be noted that the nuclei in the above figure are arranged in the sequence of increasing (N-Z)/A. Hence, a slope in ΔE is related to inadequacy of the iso-vector strength. An inspection of Figure 1 reveals that for both the parameter sets, the discrepancy between experiment and theory is maximum for ^{47}V and minimum for ^{44}Ca. Thus, the discrepancy decreases with (N-Z)/A. This analysis points towards deficiency of the SO interaction, especially, in two ways: i) the iso-scalar term is obviously too weak ii) the iso-vector term requires a substantial increase.

To further investigate the iso-vector part of the SO potential, we study the chain of Sb isotopes in the RMF framework. It should be noted that for this particular case, we solve the RMF equations without taking the currents into account. It has been shown [31] that the effect of time reversal breaking which exists in the case of odd A systems seems to cancel while taking the differences between single particle energies. Therefore, the conclusions drawn here will not change, even if the currents are explicitly taken into account.

The Sb chain gives an important clue to the iso-vector dependence of the SO potential from the spacing between single proton $2g_{7/2}$ and $1h_{11/2}$ states, revealing that the spacing E^{gh} increases with neutron number, i.e the effective SO potential for protons decreases with neutron number. Note that the single particle states $2g_{7/2}$ and $1h_{11/2}$ are less pure than the terminating states discussed above. For example, the energy spacing between $g_{7/2}$ and $h_{11/2}$ states is also influenced by quadrupole collectivity, particularly in the mid - shell region, yielding solutions that are somewhat deformed. Therefore, these states do not allow an adjustment at the same level of accuracy. Still, following the discussion in Ref. [12], the spectroscopic factors show that these states are of dominant single particle character, implying that they indeed can serve to probe both iso-scalar and iso-vector strength.

One should mention here that the increase of E^{gh} versus N is also discussed in the literature within the context of the nuclear shell-model, as being caused by the monopole part of the proton-neutron interaction and is commonly dubbed as *monopole migration* effect, see e.g. [32].According to recent investigations, the source of *monopole migration* is a two-body shell-model tensor interaction [33]. The tensor interaction can naturally be incorporated into the energy density functional framework [8, 34]. In fact, the tensor interaction has been included in the tensor interaction in the recent Skyrme - Hartree - Fock studies [35, 36, 37]. It has been shown there that it plays an important role in the evolution of the shell structure, for example, the observed trend in the $2g7/2$ - $1h11/2$ spacing. It is well known that in the mean-field approximation the two-body tensor interaction leads to a one-body SO potential, i.e. it works effectively like the two-body SO interaction. The basic difference between these two sources of one-body SO potential is that the form factor generated by the two-body tensor interaction depends on the shell-filling unlike its counterpart coming from the two-body SO interaction. In an analogous manner, the ρNN tensor coupling has been discussed for the RMF [8] generating an additional contribution to the effective one body SO potential. Hence, within the mean-field approximation, the *monopole migration* can be interpreted as a dynamical manifestation of an effec-

tive one-body SO potential. For a pedagogical discussion on this issue, see Ref. [38]. Consequently, with a suitable parameterization of the SO potential, one should be able to reproduce empirical values of E^{gh}. In Figures 2 and 3 we demonstrate that this is indeed the case by showing the results of a microscopic-macroscopic calculation with a Woods-Saxon potential, including an iso-vector term with the same sign as in RMF but considerably larger relative strength (see, for example, [39]).

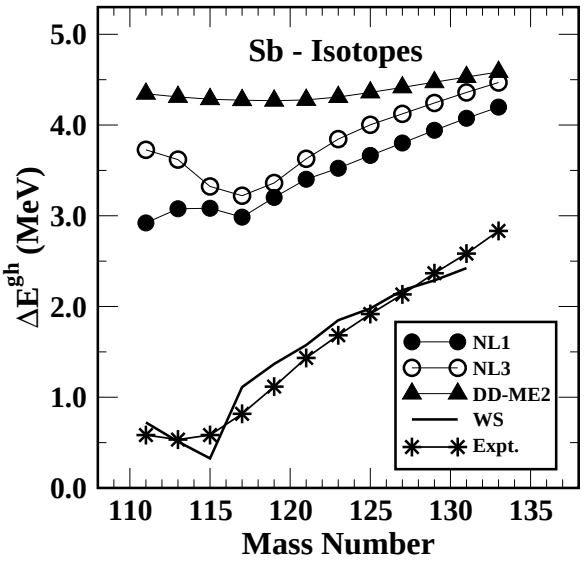

FIG. 2: The calculated and the corresponding experimental [12] E^{gh} values for Sb isotopes. Solid line marks the result of microscopic-macroscopic calculations with a Woods-Saxon potential.

The calculated and the corresponding experimental [12] values of E^{gh} are presented in Figure 2 for all the Lagrangian parameter sets considered here. The figure reveals that all the calculations deviate by large amounts from the experiment. The experimental E^{gh} varies between 0.5 MeV to around 3 MeV, whereas the corresponding calculated values (NL1 and NL3) vary within 1 MeV only. DD-ME2, on the other hand, yields almost a constant spacing. Note that the larger the calculated splitting, the smaller is the effective SO potential. The difference between the theoretical and the corresponding experimental values of E^{gh} is presented in Figure 3. This figure highlights the large deviation between theory and experiment. Interestingly, it is found that the difference decreases with increasing mass number (hence with increasing (N-Z)/A), for all the three parameter sets. This is similar to the case of ΔE (see Figure 1).

We notice again, that the effective iso-scalar SO potential in the RMF theory is too weak, yielding a much too large spacing between the $2g_{7/2}$ and $1h_{11/2}$ states. Since the iso-vector dependence of the SO is very weak in the RMF theory, with increasing (N-Z)/A, the experimental values approach the calculated ones. By increasing the coupling constants of the σ and ω meson, one

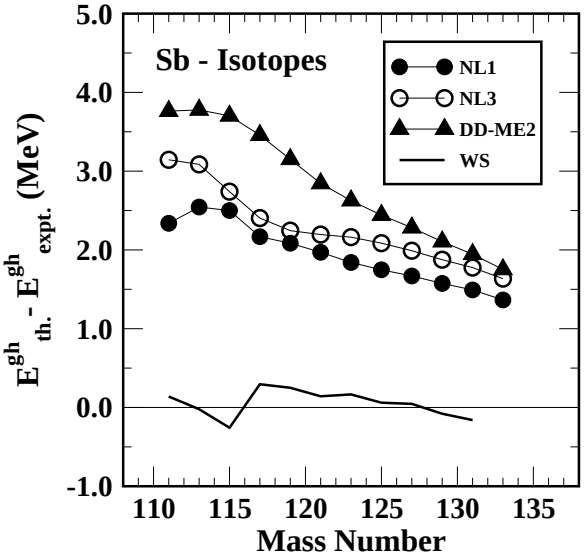

FIG. 3: The difference between the calculated and the corresponding experimental [12] E^{gh} values for Sb isotopes.

may increase the effective SO potential, and at the same time keep the central potential unchanged. However, this will only reduce the relative iso-vector strength of the SO interaction further, see Equation (2). In this way, one indeed is able to improve the effective SO potential, however, at the same time, the iso-vector potential becomes weaker. Our earlier study of the symmetry energy [40] revealed that the coupling strength of the ρ meson is rather well adjusted to reproduce the strength of the iso-vector central field. Hence, our results suggest that the presently used standard RMF Lagrangians do not allow to simultaneously adjust the iso-vector strength, i.e. increase its value in agreement to the observed experimental values and at the same time increase the SO potential. Recently, Piekarewicz [41] has studied the single particle spectra near A = 40 by adjusting m_σ and g_σ to reproduce the $1d_{3/2}$ - $2s_{1/2}$ energy gap in ^{40}Ca within the conventional RMF approach. It should be however mentioned that this is a purely localized study around A = 40. With only a few parameters in the conventional RMF, it seems rather difficult to get a good global fit that yields the correct single particle spectrum, like the gap $1d_{3/2}$ - $2s_{1/2}$ or spacing $1h_{11/2}$ - $2g_{7/2}$.

To summarize, a systematic study of the energy splitting of the terminating states between $f^n_{7/2}$ and $d^{-1}_{3/2}f^{n+1}_{7/2}$ configurations using the cranked Relativistic Mean Field theory is carried out. The principal aim of this work is to critically examine the SO potential, which emerges naturally from the RMF framework. Calculations have been carried out for NL1 and NL3 parameter sets. It is found that the one-body SO potential is essentially too weak and at the same time the experimentally observed iso-vector dependence stronger than what is found in theory. The analysis of the energy spacing between the $2g_{7/2}$ and $1h_{11/2}$ states in Sb isotopes supports these findings.

The iso-scalar part of the SO interaction is so dominant, that there is very limited freedom to improve the iso-vector SO potential generated by the ρ meson. Even the inclusion of density dependence of the meson - nucleon coupling strengths does not seem to cure this problem. Thus, it can be concluded that the standard version of the Lagrangian used, does not give enough freedom to achieve the desired strength of the SO potential and the correct iso-vector dependence in the SO interaction. This may point to the need to extend the RMF model, for example, by including tensor couplings [8] or to extend the scheme towards Hartree-Fock, including π-mesons [9].

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